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6. AUTHOR(S)
Jeng Yen and Linda Petzold

7. PERFORMING ORGANIZATION NAMES(S) AND ADDRESS(ES)
University of Minnesota
Department of Computer Science
4-192 EE/CS Bldg, 200 Union St SE
Minneapolis, MN 55455

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Convergence of the Iterative Methods for Coordinate-Splitting Formulation in Multibody Dynamics

by Jeng Yen and Linda R. Petzold

TR 95-052
July 1995
Technical Report

Computer Science Department
University of Minnesota
Twin Cities
4-192 EE/CSci Building
200 Union Street S.E.
Minneapolis, MN 55455

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Convergence of the Iterative Methods for Coordinate-Splitting Formulation in Multibody Dynamics

Jeng Yen *

Linda R. Petzold †

July 26, 1995

Abstract

In a previous paper, we introduced a *coordinate-splitting* (CS) form of the equations of motion for multibody systems which together with a modified nonlinear iteration (CM), is particularly effective in the solution of certain nonlinear highly oscillatory systems. In this paper, we examine the convergence of the CS and CM iterations and explain the improved convergence of the CM iteration. An example is given from flexible body simulation which illustrates the convergence results and the class of problems for which the CM iteration is most effective.

Keywords: constrained dynamics, multibody systems, differential-algebraic equations, numerical methods, highly oscillatory systems.

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*Department of Computer Science and Army High Performance Computing Research Center, University of Minnesota, Minneapolis, MN 55415. The work of this author was sponsored partially by the Army High Performance Computing Research Center under the auspices of the Department of the Army, Army Research Office cooperative agreement number DAAH04-95-2-0003/contract number DAAH04-95-C-0008 and by the ARO contract number DAAH04-94-G-0208, the content of which does not necessarily reflect the position or the policy of the government, and no official endorsement should be inferred.

†Department of Computer Science and Army High Performance Computing Research Center, University of Minnesota, Minneapolis, MN 55455. The work of this author was partially supported by ARO contract number DAAH04-95-C-0008, and by ARO contract number DAAL03-92-G-0247 and contract number DAAH04-94-G-0208, and by the Minnesota Supercomputer Institute.

1 Introduction

In a recent development for the solution of constrained multibody systems, we have proposed a *coordinate-splitting* (CS) formulation [24]. Numerical experiments have shown that the CS formulation is effective. In addition, its variant CM, in which the second-order derivative of the CS-projection operator is omitted in the iteration matrix, has exhibited surprisingly good results for the solution of multibody systems with high-frequency oscillations. In this paper, we present convergence results for the CS and CM method for the discretized system of equations which explain the observed behavior.

First, we give some background on the numerical solution of constrained multibody systems. For more details, we refer to [2, 6, 8, 12, 17]. The equations of motion of a constrained multibody system can be written as [10]

$$M(q)\ddot{q} - f(\dot{q}, q, t) + G(q)^T\lambda = 0 \tag{1a}$$

$$g(q) = 0 \tag{1b}$$

where $q = [q_1, q_2, ..., q_n]$ are the *generalized coordinates*, $\lambda = [\lambda_1, \lambda_2, ..., \lambda_m]$ are the *Lagrange multipliers*, $M(q) \in I\!R^{n\times n}$ is the mass-inertia matrix, $f \in I\!R^n$ is the force applied to the system, $\dot{q} = \frac{dq}{dt}$ is the velocity and $\ddot{q} = \frac{d^2q}{dt^2}$ is the acceleration vector. The constraints $g = [g_1, g_2, ..., g_m]$ are m smooth functions of q, whose Jacobian

$$G(q) = \left[\frac{\partial g_i}{\partial q_j}\right] \in I\!R^{m\times n}\ ,\ m \le n \tag{2}$$

is assumed of full row-rank. We also assume that $G(q)M(q)G^T(q)$ is symmetric and positive definite for every $q \in I\!R^n$ to obtain a consistent physics represented by (1). The *degrees of freedom* for the system (1) is then p, where $p = n - m$.

It is useful to note that, for a *conservative* system, the *constraint reaction force* $G^T\lambda$ in (1a) is obtained by the derivative of *reduced potential energy* [15]

$$V^r(q) = \lambda^T g(q) \tag{3}$$

for every solution of λ and q from (1). Differentiating Eq. (1b) yields the velocity constraints,

$$G(q)v = 0 \tag{4}$$

and differentiating Eq. (4) gives the acceleration constraints,

$$G(q)\dot{v} + \frac{\partial(Gv)}{\partial q}v \equiv G(q)\dot{v} - \gamma(v, q) = 0. \tag{5}$$

To eliminate the constraints, we may choose m coordinates of $q = Xx + Yy$ such that $(G(q)Y)^{-1}$ exists in a neighborhood of q, where $X \in \mathbb{R}^{n\times p}$ and $Y \in \mathbb{R}^{n\times m}$, whose columns constitute the standard basis for $\mathbb{R}^n$. Since $G(q)$ is full-rank, we can use the splitting of $q = Xx + Yy$ to obtain a linear operator defined as follows:

Definition 1 *[Coordinate-Splitting Matrix] Let X and Y be the matrices whose columns constitute the standard basis of $\mathbb{R}^{n\times n}$ such that $\|(G(q)Y)^{-1}\|$ is bounded in a neighborhood U_0 of q_0. The $p \times n$* coordinate-splitting matrix *for (1) is defined by*

$$P(q) = X^T - Q(q)^T Y^T = X^T(I - G(q)^T(G(q)Y)^{-T}Y^T) \tag{6}$$

where $Q(q) = (G(q)Y)^{-1}G(q)X$.

Remark 1 *From the construction of the CS matrix $P(q)$, we can easily see that $P(q)G^T(q) = 0$ for all $q \in \mathbb{R}^n$, i.e., $P(q)$ is orthogonal to range(G^T). Furthermore, the row vectors of $P(q)$ are orthonormal, i.e., $P(q)^T P(q) = I_p$ where I_p is the identity matrix in $\mathbb{R}^p$.*

Reducing (1) to a first-order DAE, appending the velocity constraints (4) to (1), and applying $P(q)$ to its differential part, we obtain an index 1 DAE

$$\begin{aligned} P(q)(\dot{q} - v) &= 0 && (7a)\\ P(q)(M(q)\dot{v} - f(v,q,t)) &= 0 && (7b)\\ G(q)v &= 0 && (7c)\\ g(q) &= 0. && (7d) \end{aligned}$$

Note that one can use the *generalized coordinate partitioning method* to reduce (1) to the p differential equations [22]

$$\hat{M}(x, h(x))\ddot{x} = \hat{f}(\dot{x}, \frac{dh}{dx}\dot{x}, x, h(x), t) \tag{8}$$

where $h(x)$ is the implicit function of y defined by the constraints. The equation (8) is equivalent to the *underlying state-space* form of the coordinate-splitting formulation (7) of the constrained multibody systems. However, the function $h: \mathbb{R}^p \to \mathbb{R}^m$ and its time derivative cannot be evaluated unless the constraint equations (1b) and their derivatives have been satisfied, e.g., the computations of $\hat{M}$ and $\hat{f}$ require $(x, h(x))$ to lie on the constraint manifold

$$\mathcal{M} = \{q \in \mathbb{R}^n \mid g(q) = 0\}$$

and $(\dot{x}, \frac{dh}{dx}\dot{x})$ a tangent vector to $\mathcal{M}$ at $(x, h(x))$. These conditions necessitate the solution of the nonlinear constraint equations and their derivatives. The numerical solution of (8) can be inefficient when $\hat{f}$ is *stiff*, even if implicit numerical integration methods are applied, because of the computational complexity of $h(x)$, $\hat{f}$, and their derivatives.

In any case, it is advantageous to use (7) rather than (8) for the numerical solution of (1), because there is less computational complexity to obtain (7) than (8). Applying numerical integration to (7), we will show in Sec. 2 that the CS and CM iterations solve the nonlinear system (7) efficiently in a two-stage iteration. First, we carry out the iteration of a $2n \times 2n$ system of the Newton-Euler equations with some additional terms corresponding to the derivative of the reduced potential (3). Then, we solve for the increments of the *dependent coordinate* y holding the *independent coordinate* fixed on the range space of the projection operator, and finally update the factorization of the $m \times n$ constraint Jacobian G. For the CM iteration, the first iteration of the $2n \times 2n$ Newton-Euler equations (7a) and (7b) uses only their unconstrained form, e.g., the second-order derivatives are omitted.

In Sec. 3, we show the convergence of the CS and CM iterations under a moderate assumption on the smoothness of the constraint manifold $\mathcal{M}$. For a sufficient condition of the convergence, we give a required stepsize of the numerical integration methods. The sufficient conditions of the numerical integration for the CS and CM iterations are different, given the same starting values of the iterations. For problems with a small potential energy force, e.g., $\nabla V^r(q) \equiv \frac{dV^r}{dq}$ is small, the CM iteration is advantageous over the CS iteration. As shown in [24], the CM iteration has not only less computational complexity, but also better convergence for the bushing example, compared to the CS iteration.

In the presence of highly oscillatory forces, the stepsize h of the numerical integration may be restricted to $h \leq \sqrt{\|\frac{\partial f}{\partial q}\|^{-1}}$ if one will resolve all the high-frequency oscillations. Here, we are not interested in small oscillations with high-frequency, hence we used a discretization method with strong damping properties and the stepsize h is *not* restricted by the high-frequency oscillations of an amplitude smaller than the error tolerance. However, the convergence of the Newton iteration for (7) is subject to a good approximate Jacobian at the predicted solution. Since for the highly oscillatory mechanical systems, the Jacobian evaluated at a predicted solution may be far away from the Jacobian at the corresponding numerical solution, the Newton iteration for the discretized nonlinear equations has convergence difficulties. For some model problems, while the stepsize in the CS iteration must be restricted to obtain Newton convergence, it is not the case in the CM iteration. Using a simplified Newton iteration, we analyze the rate of convergence for the CS and CM iterations in Sec. 4 and explain the different convergence behavior for the highly oscillatory case.

In modeling a *deformable* body, the most commonly used technique is the *finite element* method, which yields linear deformation forces in the body-fixed local coordinate systems. We illustrate that the theorem in Sec. 4 can be applied to this class of constrained multibody systems and predicts the results. We re-examine the 2D bushing problem in Sec. 5.

2 Solving the nonlinear system

In this section, we examine the iterative solution of the CS formulation and its variant, the CM iteration. Denoting the current time $t = t_n$ and (q_n, v_n) the numerical solution, applying for example a BDF formula to (1) yields

$$\begin{aligned} P(q_n)(\rho_h q_n - v_n) &= 0 && \text{(9a)} \\ P(q_n)(M(q_n)\rho_h v_n - f(v_n, q_n, t_n)) &= 0 && \text{(9b)} \\ G(q_n)v_n &= 0 && \text{(9c)} \\ g(q_n) &= 0 && \text{(9d)} \end{aligned}$$

where ρ_h is the discretization operator. We will investigate Newton-type methods for the solution of (9). To form the Jacobian, we will need to find the derivative of a vector function in the form of $P(q)r$ with respect to q. In [24], it was shown that this can be written as

$$\frac{d}{dq}(P(q)r) = P(q)\frac{dG^T(q)s}{dq} \qquad \text{with} \qquad s = (G(q)Y)^{-T}Y^T r. \tag{10}$$

Using the product rule, we obtain the derivative of $P(q)r(q)$,

$$\frac{d}{dq}(P(q)r(q)) = P(q)[\frac{dr(q)}{dq} + \frac{dG^T(q)s}{dq}] \tag{11}$$

where s is the same as in (10). Thus, for a given CS matrix at q, the vector function $P(q)r(q)$ is differentiable with the order no less than the minimum between those of $r(q)$ and $G(q)$.

Using (11), and denoting $r_1 = \rho_h q_n - v_n$ and $r_2 = M(q_n)\rho_h v_n - f(v_n, q_n, t_n)$, the Jacobian of (9) is

$$J(q_n, v_n) = \begin{bmatrix} P(q_n)[\frac{\partial G(q_n)^T s_1}{\partial q_n} + \frac{\partial \rho_h q_n}{\partial q_n}] & -P(q_n) \\ P(q_n)[\frac{\partial G(q_n)^T s_2}{\partial q_n} + \frac{\partial r_2(q_n, v_n)}{\partial q_n}] & P(q_n)\frac{\partial r_2(q_n, v_n)}{\partial v_n} \\ \frac{\partial (G(q_n)v_n)}{\partial q_n} & G(q_n) \\ G(q_n) & 0 \end{bmatrix} \tag{12}$$

where $s_1 = (GY)^{-T}Y^T r_1$ and $s_2 = (GY)^{-T}Y^T r_2$. The Newton equations of the discretized form of (9) are

$$
\begin{aligned}
P_n\left(\left[\frac{d\rho_h q_n}{dq_n} + \frac{d(G_n^T s_1)}{dq_n}\right]\Delta q_n - \Delta v_n\right) &= -P_n r_1 && \text{(13a)}\\
P_n\left(\left[\frac{\partial(M_n\rho_h v_n - f_n)}{\partial q_n} + \frac{d(G_n^T s_2)}{dq_n}\right]\Delta q_n + \frac{(M_n d\rho_h v_n - f_n)}{dv_n}\Delta v_n\right) &= -P_n r_2 && \text{(13b)}\\
\frac{dG_n v_n}{dq_n}\Delta q_n + G_n\Delta v_n &= -G_n v_n && \text{(13c)}\\
G_n\Delta q_n &= -g_n && \text{(13d)}
\end{aligned}
$$

at the time $t = t_n$, where Δq_n and Δv_n are the increments of q_n and v_n by the Newton iterations. For notational simplicity, we write the subscript n of a function representing its numerical value at t_n, e.g., $g_n = g(q_n)$.

A modification of the iteration matrix (12) leads to the CM method as explained in the following. Combining (13a) and (13b), we obtain

$$
\begin{bmatrix} P(q_n) & 0 \\ 0 & P(q_n) \end{bmatrix} \left(J_1(q_n, v_n) \begin{bmatrix} \Delta q_n \\ \Delta v_n \end{bmatrix} + \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} \right) = 0 \tag{14}
$$

where the $2n \times 2n$ matrix J_1 is

$$
J_1(q_n, v_n) = \begin{bmatrix} \frac{d\rho_h q_n}{dq_n} + \frac{d(G_n^T s_1)}{dq_n} & -I \\ \frac{d(M(q_n)\rho_h v_n)}{dq_n} - \frac{\partial f_n}{\partial q_n} + \frac{d(G_n^T s_2)}{dq_n} & M\frac{d\rho_h v_n}{dv_n} - \frac{\partial f_n}{\partial v_n} \end{bmatrix}. \tag{15}
$$

Replacing $\frac{dP(q)r(q)}{dq}$ by $P(q)\frac{dr(q)}{dq}$, i.e., fixing the CS operator, (15) yields

$$
\bar{J}_1(q_n, v_n) = \begin{bmatrix} \frac{d\rho_h q_n}{dq_n} & -I \\ \frac{d(M(q_n)\rho_h v_n)}{dq_n} - \frac{\partial f_n}{\partial q_n} & M\frac{d\rho_h v_n}{dv_n} - \frac{\partial f_n}{\partial v_n} \end{bmatrix} \tag{16}
$$

where the second-order derivatives $\frac{dG^T s_1}{dq}$ and $\frac{dG^T s_2}{dq}$ in (15) are nullified. Replacing the Jacobian matrix $J_1(q_n, v_n)$ by this approximate Jacobian matrix $\bar{J}_1(q_n, v_n)$ in the iteration, we defined the CM iteration [24].

The iterative solutions of CS or CM for (9) require the solution of the linear system (13), which can be obtained from one additional matrix factorization, i.e., the factorization of (15) or (16). Since J_1 is generally invertible under the assumption of $M(q_n)$ nonsingular, one solution of (14) can be computed by

$$
\begin{aligned}
(X^T - Q_n^T Y^T)(\Delta q_n - \hat{r}_1) &= 0 && \text{(17a)}\\
(X^T - Q_n^T Y^T)(\Delta v_n - \hat{r}_2) &= 0 && \text{(17b)}
\end{aligned}
$$

where

$$
J_1(q_n, v_n) \begin{bmatrix} \hat{r}_1 \\ \hat{r}_2 \end{bmatrix} = \begin{bmatrix} -r_1 \\ -r_2 \end{bmatrix}. \tag{18}
$$

Note that (17a) is not a necessary but a sufficient condition of the solution of (14). Then, we solve (17a) and (13d) for Δq_n. Using Δq_n to compute $\frac{dGv}{dq}(q_n)\Delta q_n$, we solve (17b) and (13c) for Δv_n. The solution $(\Delta q_n, \Delta v_n)$ requires only solving two linear systems of the form

$$\begin{bmatrix} P \\ G \end{bmatrix} u = \begin{bmatrix} a \\ b \end{bmatrix} \tag{19}$$

for $u \in I\!R^n$, $a \in I\!R^p$, and $b \in I\!R^m$. Denoting $u = Xu_x + Yu_y$, we obtain from the first p equations of (19)

$$u_x - Q^T u_y = a \tag{20}$$

and the second m equations yield

$$u_y = (GY)^{-1}(b - (GX)u_x). \tag{21}$$

Substituting (21) into (20) and solving for u_x yields

$$u_x = (I_p + Q^T Q)^{-1}(a + Q^T (GY)^{-1} b) \tag{22}$$

where I_p is the $p \times p$ identity matrix. According to (21) and (22), the solution of (19) depends only on its independent part, e.g., u_x.

Combining (17a) with (13d), we obtain

$$\begin{aligned} \Delta x_n &= -(I_p + Q_n^T Q_n)^{-1}(-X^T \hat{r}_1 + Q_n^T (Y^T \hat{r}_1 - (G_n Y)^{-1} g_n)) && \text{(23a)} \\ \Delta y_n &= -(G_n Y)^{-1}(g_n + (G_n X)\Delta x_n) && \text{(23b)} \end{aligned}$$

and from (17b) and (13c), we have

$$\begin{aligned} \Delta w_n &= -(I_p + Q_n^T Q_n)^{-1}(-X^T \hat{r}_2 + Q_n^T (Y^T \hat{r}_2 - (G_n Y)^{-1} \eta_n)) && \text{(24a)} \\ \Delta z_n &= -(G_n Y)^{-1}(\eta_n + (G_n X)\Delta w_n) && \text{(24b)} \end{aligned}$$

where $\eta_n = \frac{d(Gv_n)}{dq}\Delta q_n$, and $v_n = Xw_n + Yz_n$. The numerical solutions (23) and (24) illustrate that the dependent variables y_n and z_n are determined geometrically, e.g., use only the algebraic constraints. Therefore, applying numerical integration to q_n and v_n, the local errors can be bounded by the difference in x_n and w_n using CS or CM iterations.

It is useful to examine the difference between the CS and CM iterations. The components of J_1 that are dismissed by the CM iteration represent the derivative of the CS matrix $P(q)$, that is, the tensor of the second-order derivative of the constraint equations. The influence of this tensor on the increment Δq may be expressed by

$$\frac{d}{dq}(P(q)r)\Delta q = -P(q)[\frac{dG(q)^T \Delta\hat{y}}{dq}]r \tag{25}$$

where $\Delta\hat{y} = (GY)^{-T}Y^T\Delta q$. The exchange of Δq and r in (25) is permitted by the smoothness of the constraint manifold defined by $\mathcal{M} = \{q \in I\!R^n | g(q) = 0\}$, on which $\frac{d}{dq}G^T(q)(GY)^{-T}Y^T$ is a bilinear form. The term (25) measures the rate of change of the normal vector $G^T\Delta\hat{y}$ (to the constraint manifold at q) along the solution curve on the independent generalized coordinate space. The difference between the CS and CM iterations can be expressed in terms of (25) with the corresponding residual vectors r_1 and r_2 of (13a) and (13b), respectively.

3 Convergence of CS and CM Iterations

The convergence results for the CS and CM iterations can be carried out on a smooth constraint manifold $\mathcal{M}$. We assume that for any $q_0 \in \mathcal{M}$, there exist $X \in I\!R^{p\times n}$ and $Y \in I\!R^{m\times n}$ such that

$$\|(G(q)Y)^{-1}\| \leq C_1 \tag{26}$$

$$\|G(q_1)^T - G(q_2)^T\| \leq C_2\|q_1 - q_2\| \tag{27}$$

for some C_1 and C_2, where q, q_1, and q_2 are in a neighborhood $U(q_0)$ of q_0.

Remark 2 *The matrices X and Y for a given q_0 may be selected according to different strategies. For instance, applying Gaussian elimination with row pivoting to $G^T(q_0)$, one obtains Y by the permutation indices of the factorized matrix. In this case, C_1 of (26) is the same order of magnitude as $\|(GG^T)^{-1}\|$. On the other hand, C_2 of (27) is the Lipschitz constant of G, which is independent of the choice of X and Y.*

With the conditions (26) and (27), it is easy to obtain an upper bound for the difference term (25) between the CS and the CM iterations.

Lemma 1 *Suppose conditions (26) and (27) hold. Then*

$$\|\frac{d}{dq}[P(q)r(q)] - P(q)\frac{dr(q)}{dq}\| \leq R_0C_1C_2\|Y^Tr(q)\| \tag{28}$$

in $D(q_0, R_0) \subseteq U(q_0)$, where $D(q_0, R_0)$ is the disc in $I\!R^n$ with center q_0 and radius R_0.

Proof. The inequality is a direct consequence of (10) and (11). Subtracting (10) from (11) and taking the norm of the remainder yields

$$\|\frac{d}{dq}[P(q)r(q)] - P(q)\frac{dr(q)}{dq}\| = \|P(q)\frac{dG(p)^T(GY)^{-1}Y^Tr}{dq}\|.$$

Since the row vectors of $P(q)$ are p orthonormal vectors in $\mathbb{R}^n$, applying the Cauchy inequality gives

$$\|P(q)\frac{dG(p)^T(GY)^{-1}Y^Tr}{dq}\| \leq \|\frac{dG(q)^Ts}{dq}\| \leq R_0C_2\|(GY)^{-T}Y^Tr(q)\|$$

for all $q \in D(q_0, R_0) \subseteq U(q_0)$. Condition (26) implies the result in (28). □

For simplicity we now consider, instead of the second-order constrained equations of motion (1), a first-order system of

$$\dot{q} - f(q,t) + G^T\lambda = 0 \qquad (29a)$$
$$g(q) = 0 \qquad (29b)$$

since the convergence results of CS and CM methods for (29) can be trivially extended to (1). Applying coordinate-splitting to (29) at the time $t = t^*$, we obtain the nonlinear equations

$$F(q^*) = \begin{bmatrix} P(q^*)r(q^*) \\ g(q^*) \end{bmatrix} \qquad (30)$$

where the *residual* function is

$$r(q,t) = \rho_h(q) - f(q,t), \qquad (31)$$

using the linear discretization operator ρ_h with the time step h. Denoting the numerical solution of the nonlinear equations (30) by q^*, and the numerical solution of (31) by $\tilde{q}^*$ at the time $t = t^*$ we apply the theorem of Newton-Kantorovich to the CS iteration, yielding the convergence of CS [5].

Theorem 1 (Convergence of CS iteration) *Suppose conditions (26) and (27) hold at the solution q^* of (30) for a selected Y. Applying multistep numerical integration, if the numerical discretization operator ρ_h satisfies*

$$\| \left(\frac{dr}{dq} + \frac{dG^Ts}{dq}\right)^{-1} \| \leq C_0 < 1 \qquad (32)$$

with $s = (GY)^{-T}Y^Tr$, for all $q \in U(\tilde{q}^*)$, where the numerical solution $\tilde{q}^*$ of (31) is sufficiently close to q^*, e.g., $q^* \in U(q^*) \cap U(\tilde{q}^*)$, then for all starting values q_0 such that $\|q^* - q_0\| \leq R_0$ for some $R_0 > 0$, the sequence $\{q_k\}$ generated by

$$q_{k+1} = q_k - J(q_k)^{-1}F(q_k) = q_k - \begin{bmatrix} P(q_k)(r_q(q_k) + \frac{dG(q_k)^Ts_k}{dq}) \\ G(q_k) \end{bmatrix}^{-1} F(q_k) \qquad (33)$$

where $r_q = \frac{dr}{dq}$ and $s_k = (G(q_k)Y)^{-T}Y^Tr(q_k)$, converges to q^*.

Proof. Under the assumptions, the Jacobian matrix $J(q^*)$ of the equations (30) is nonsingular, $G(q)$ is Lipschitz continuous, and $\|(\frac{d}{dq}(r+G^Ts))^{-1}\| \leq C_0 < 1$ in $U(q^*) \cap U(\tilde{q}^*)$. Thus $J(q)$ is Lipschitz continuous and $J(q^*)^{-1}$ is bounded. Therefore, $\{q_k\}$ defined by (33) will converge if the initial guess q_0 is sufficiently close to q^*. This is a standard proof of convergence of the Newton method for (30). For details we refer to [5], pp. 90-91. □

Remark 3 *The assumption $q^* \in U(q^*) \cap U(\tilde{q}^*)$ and the existence of J^{-1} depend on the time steps h, of (31). Since the time step is not the focus here, we will assume an appropriate h for ρ_h in all the discussions. In general, we may obtain*

$$\|q^* - \tilde{q}^*\| \leq \min\{C_0\|r(q^*)\|, C_1\|g(\tilde{q}^*)\|\} \leq O(h^j)$$

for some j consistent with the order of discretization operator ρ_h, since

$$\|q^* - q(t^*)\| \leq O(h^j) \;\; and \;\; \|\tilde{q}^* - q(t^*)\| \leq O(h^j)$$

where $q(t^*)$ is the analytical solution of (29). The R_0 in Theorem 1 may be taken to be

$$R_0 \leq \frac{1}{2\|J^{-1}\|\|\frac{dJ(q)}{dq}\|}.$$

For convergence, one of the sufficient conditions for the above theorem requires that the numerical integration satisfies (32). This implies that the stepsize h has an upper bound. For linear multistep integration, e.g., $\frac{\partial \rho_h(q)}{\partial q} = \frac{\alpha}{h}$, the stepsize must satisfy

$$\frac{h}{\alpha}\|\left(I - \frac{h}{\alpha}\frac{\partial}{\partial q}(f - G^Ts)\right)^{-1}\| \leq 1 \tag{34}$$

where α is the leading coefficient of the numerical integration formula. Convergence of the CM iteration can also be assured for a sufficiently accurate initial guess. Carrying out the CS iteration (33), the increment $\Delta q_k \in \mathbb{R}^n$ satisfies

$$P(q_k)\left(r_q(q_k) + \frac{dG(q_k)^Ts_k}{dq}\right)\Delta q_k = -P(q_k)r(q_k) \tag{35a}$$

$$G(q_k)\Delta q_k = -g(q_k) \tag{35b}$$

at the kth iteration. The corresponding CM solution at the kth iteration yields

$$P(q_k)r_q(q_k)\Delta\bar{q}_k = -P(q_k)r(q_k) \tag{36a}$$

$$G(q_k)\Delta\bar{q}_k = -g(q_k). \tag{36b}$$

A bound on the difference between $\Delta\bar{q}_k$ and Δq_k can be computed and convergence of the CM iteration can be shown as follows.

Lemma 2 *Suppose conditions (26), (27) and*

$$\left\| \left(\frac{dr}{dq}\right)^{-1} \right\| = \left\| \left(\frac{d\rho_h}{dq} - \frac{\partial f}{\partial q}\right)^{-1} \right\| \le C_0 < 1 \tag{37}$$

hold in a neighborhood of q^*, and

$$\bar{J}(q^*) = \begin{bmatrix} P(q^*)r_q(q^*) \\ G(q^*) \end{bmatrix}$$

is invertible. Let $\{q_k\}$ generated by the CS iterations converge to q^*, and $\Delta\bar{q}_k$ be the solution of the CM iteration at q_k for $k = 0, 1, 2, \ldots$. Then $\{\delta q_k = \Delta q_k - \Delta\bar{q}_k\}$ satisfies

$$\|\delta q_k\| \le R_0 C_1 C_2 \|\bar{J}^{-1}(q^*)\| \|Y^T r(q^*)\| \|\Delta q_k\| = O(h^j) \tag{38}$$

using a jth-order numerical integration method, for some $k \ge K_1 > 0$, for K_1 sufficiently large.

Proof. Subtracting (35) from (36) yields

$$\bar{J}(q_k)\delta q_k = -\begin{bmatrix} P(q_k) \\ 0 \end{bmatrix} \frac{dG(q_k)^T (GY)^{-T} Y^T r_k}{dq_k} \Delta q_k$$

where

$$\bar{J}(q_k) = \begin{bmatrix} P(q_k)r_q(q_k) \\ G(q_k) \end{bmatrix}.$$

This implies

$$\|\delta q_k\| \le \|\bar{J}^{-1}(q_k)\| \left\| P(q_k) \frac{dG(q_k)^T (GY)^{-T} Y^T r_k}{dq_k} \right\| \|\Delta q_k\|.$$

Using (28), for any $k \ge K_0$, the first term of the right-hand side of (38) is obtained by (28). To show that this term is actually $O(h^j)$, we note that $\|\Delta q_k\| = O(h^j)$ for k sufficiently large, since $\|F_k\| \to 0$ when $k \to \infty$. □

Theorem 2 (Convergence of CM iteration) *Under the conditions in Lemma 2, choosing $\bar{q}_0 = q_0$, the sequence $\{\bar{q}_k\}$ generated by the CM iterations*

$$\bar{q}_{k+1} = \bar{q}_k - \bar{J}(\bar{q}_k)^{-1} F(\bar{q}_k) \tag{39}$$

converges to $\bar{q}^*$ and

$$\|\bar{q}^* - q(t^*)\| \le O(h^j). \tag{40}$$

Proof. Since $\bar{J}$ is nonsingular and its components are smooth functions, using (21) and (22), we can write

$$\bar{J}^{-1} = \begin{bmatrix} I_p + Q^T Q & 0 \\ -Q & I_m \end{bmatrix}^{-1} \begin{bmatrix} I_p & Q^T(GY)^{-1} \\ 0 & (GY)^{-1} \end{bmatrix} \begin{bmatrix} \frac{dr}{dq} \end{bmatrix}^{-1}$$

for the CM iteration, providing $\frac{dr}{dq}$ is invertible. By conditions (26) and (27), we have

$$\| \begin{bmatrix} I_p + Q^T Q & 0 \\ -Q & I_m \end{bmatrix}^{-1} \| \leq C_3$$

and

$$\| \begin{bmatrix} I_p & Q^T(GY)^{-1} \\ 0 & (GY)^{-1} \end{bmatrix} \| \leq C_4$$

for some constants C_3 and C_4. Thus, the contractive condition (37) implies convergence of the CM iteration. □

Note that (37) for the CM method is analogous to (32) for the CS method. Instead of (34) for multistep integration methods using the CS iteration, the stepsize condition for the CM iteration is given by

$$\frac{h}{\alpha} \| \left(I - \frac{h}{\alpha} \frac{\partial f}{\partial q} \right)^{-1} \| \leq 1 \tag{41}$$

in accordance with (37).

Remark 4 *The sufficient condition (41) is not a necessary condition for the convergence of the CM iteration. If the CM iteration is carried out by the solution of (18) followed by (19), then the stepsize condition (41) can be rewritten as*

$$\frac{h}{\alpha} \| \left(I - \frac{h}{\alpha} P(q^*) \frac{\partial f}{\partial q}(q^*) \right)^{-1} \| \leq 1.$$

It is easy to see that $\{q_k\}$ of the CS iterations and $\{\bar{q}_k\}$ of the CM iterations are the same if g is linear in q. In general, the rate of convergence of the CM iteration is *superlinear*, using the Dennis-Moré Characterization Theorem [7]. Moreover, if the constraints are actually invariant to the differential equations, i.e., $\lim_{h \to 0} r(q^*) = 0$, then we have $\bar{J}(q^*) = J(q^*)$.

It is noteworthy that the CS iteration can also be implemented in the stabilized DAE formulations, which are based on the application of the method of Lagrange multipliers [24]. For example, we have considered the stabilized index-2 form [8]. The

algebraic variables are obtained from the solution of s_1 and s_2 in the computation of the Jacobian (12). Analogous to the CM modification, we can eliminate the second-order derivative of the reaction forces, e.g., $G^T\lambda$ in (1b), yielding an approximate Jacobian similar to that of the CM iteration. However, additional modifications to the convergence test of the Newton iteration for the Lagrange multiplier based formulation are required. For the Newton convergence, a similar result to Theorem 4 holds for the Lagrangian formulations in certain problems, but the modified convergence test is no longer reliable.

4 Rate of convergence for highly oscillatory multi-body systems

One challenging class of problems in multibody dynamic systems (MBS) is the solution of systems with high-frequency vibration. High frequency oscillatory forces often appear in the modeling of vehicle suspension systems, modal analysis in structural dynamics, or modeling oscillations in computer-aided engineering etc. Using the CS formulation, we may write the oscillatory equations of motion as

$$\begin{aligned} P(q)(\dot{q}-v) &= 0 && \text{(42a)} \\ P(q)(M(q)\dot{v}+\frac{1}{\epsilon}\eta(q)-f(v,q,t)) &= 0 && \text{(42b)} \\ g(q) &= 0 && \text{(42c)} \\ G(q)v &= 0 && \text{(42d)} \end{aligned}$$

where $\frac{1}{\epsilon}$ may be, for example, the coefficients of stiff springs; i.e., $0<\epsilon\ll 1$. In practice, $\eta(q)$ is usually oblique towards $Ker P(q)$, i.e., the oscillatory force(s) act on both the independent and the dependent coordinates. For the numerical solution of (42), experiments have shown that the CM iteration performed superior to the CS iteration [24] for those types of problems. For the purpose of obtaining a smooth solution with large stepsizes [18], we can explain the reason why the CM iteration is so effective.

In the modeling of deformable multibody systems, the nonlinear oscillatory forces in (42b) are usually derived from the theory of linear elasticity, i.e., for some functions $\tilde{q}$ such that the oscillatory forces may be written as $\frac{1}{\epsilon}\tilde{q}$. We can use these functions $\tilde{q}$ to write the nonlinear force, e.g.

$$\frac{1}{\epsilon}\eta(q)=\frac{1}{\epsilon}\tilde{q},$$

and then append

$$\tilde{q} - \eta(q) = 0$$

to the constraint equations. The oscillatory forces will then become *linear* with respect to the variables $\tilde{q}$. In fact, if the oscillatory forces were produced by a finite element approximation of the deformation of bodies, components of $\tilde{q}$ are associated with some body-fixed local coordinates via the orientation transformation matrix, whose entries often are slowly varying in time.

Deformation forces are the most common potential forces that can produce small amplitude high-frequency oscillations, and they are usually linear with respect to the local coordinates [4, 25]. For these reasons, we will consider the class of oscillatory forces in the form

$$\eta(q) = B(t)(q - b_0(t)) \tag{43}$$

where components of B and b_0 are slowly varying. In particular, B and b_0 may be functions of some constraint-driven generalized coordinates. For example, $B(\theta)$ in the 2D bushing problem in [24] has the form

$$B(\theta) = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} k^x & 0 & 0 \\ 0 & k^y & 0 \\ 0 & 0 & k^\theta \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}^T \tag{44}$$

where θ is small, and k^x, k^y and k^θ are positive constants.

Using a linear oscillatory force, the Lagrange equations of motion of the MBS can be written as

$$M(q)\dot{v} + \frac{1}{\epsilon}B(q - b_0) + G^T\lambda - f(v, q, t) = 0 \tag{45}$$

where $\frac{1}{\epsilon} \gg \|\frac{\partial f}{\partial(q,v)}\|$. From the assumption (27) of the constraint manifold, we can also see that

$$\frac{1}{\epsilon} \gg \max_{\|u_1\|,\|u_2\|=1} \|\frac{dG(q)u_1}{dq}u_2\| \tag{46}$$

for all q.

In the context of the *CS* formulation, the problem of convergence of the Newton iteration can be explained by analyzing the *reduced potential* function. The *reduced potential* of (42b) is

$$V^r(q) = g(q)^T(GY)^{-T}Y^Tr \tag{47}$$

where $r = f - M\tilde{q} - \frac{1}{\epsilon}B(q - b_0)$. The *reduced potential force* generated by (47) is

$$\nabla V^r(q) \equiv \frac{dV^r}{dq} = G^T(GY)^{-T}Y^Tr. \tag{48}$$

At each iteration, the reduced potential force acts along the *normal* direction of the constrained manifold enforcing the constraint equations. The gradient of the correction term yields

$$\nabla^2 V^r(q) = (I - G^T(GY)^{-T}Y^T)\frac{dG^T(q)s}{dq} \tag{49}$$

where $s = (GY)^{-T}Y^T r$. Applying Y^T to (49), gives

$$Y^T\nabla^2 V^r(q) = Y^T(I - G^T(GY)^{-T}Y^T)\frac{dG^T(q)s}{dq} = 0$$

and applying X^T to (49) yields

$$X^T\nabla^2 V^r(q) = P(q)\frac{dG^T(q)s}{dq}.$$

When high-frequency oscillations appear in the system, e.g., $\epsilon \rightarrow 0$, the reduced potential force also becomes oscillatory if $Y^T r$ is nonzero. This is the general case when the solution is not at an equilibrium position. Nevertheless, convergence of the CS iteration can be achieved by using a small enough stepsize, e.g., $h \approx \sqrt{\epsilon}$.

Theorem 3 *Let (q, v) be the solution of the nonlinear system (42), which results from numerical integration using ρ_h with a stepsize h. Suppose the starting value (q_0, v_0) satisfies $\|q_0\| = O(h^2)$ and $\|v_0\| = O(h)$, and $J(q_0)$ is nonsingular. Then the CS iteration converges if $h^2 \leq c\epsilon$ for some moderate c.*

Proof. For the convergence of the CS iteration, we need to show that (32) is valid, where $r(q)$ is defined in (45). For (32), we have

$$\|\frac{\partial r}{\partial q}(q_0) + \frac{dG^T s}{dq}(q_0)\| = \|\frac{\alpha\|M\|}{h^2} - \frac{1}{\epsilon}\| + O(h)$$

where $\alpha > 0$ is the leading coefficient of ρ_h, and $\|M\|$ is not zero. Consequently, for $\epsilon \ll 1$, (32) is valid provided that $h \approx \sqrt{\epsilon}$. $\square$

From the above theorem, we can obtain the same convergence result for the CM iteration using Lemma 2, provided $\bar{J}(q_0)$ is invertible. In many applications, following the oscillations is *not* of interest. Instead, one wants to use a large time step to damp out the oscillations of small amplitude but high frequency. For this reason, we now consider only the multistep numerical integration methods that are *strictly stable* at infinity and A-stable, such as the lower order (i.e., ≤ 2) BDF methods [12]. The convergence of L-stable implicit Runge-Kutta methods to the *smooth* solution of

highly oscillatory ODE of multibody mechanical systems can be found in [18]. Here we focus on the convergence of the CM iteration for constrained multibody systems with oscillatory forces when applying the above-mentioned linear multistep methods.

Numerical solutions on the *slow manifold* can be evaluated using the equilibrium of (42b), i.e., the *slow* solution [1, 14] satisfies

$$\eta(q) - \epsilon(f(v,q) - \nabla V^r(q) - M(q)\dot{v}) = 0,$$

and the *smooth* solution is its asymptotic expansion to some order of ϵ around the manifold $\{q \mid \eta(q) = 0\}$. In the linear form, the smooth solution of (42) is not far from $B(q - b_0) = 0$ since $\frac{1}{\epsilon} \gg \|\frac{\partial f}{\partial(q,v)}\|$. For the strongly damped numerical solution q_n, $B(q_n - b_0) \rightarrow O(\epsilon)$ as $t_n \rightarrow \infty$. During the iterative solution onto the *slow manifold*, the constraints may not be satisfied, which causes a large reaction force in the form of (48). This may cause oscillations in the CS iteration, while the CM iteration annihilates these nonlinear oscillations generated by the reduced potential. This yields a superior performance of the CM iteration as compared to the CS iteration for computing the smooth solution of (42). The result is explained in the following.

Lemma 3 *Let (q^*, v^*) be the smooth solution of (42), $\eta(q)$ linear, and h the stepsize of the multistep integration method. Suppose the starting values (q_0, v_0) for (q^*, v^*) on the smooth solution of (42), i.e., $\|q^*\| = O(\epsilon)$ and $r(q^*, v^*) = O(h)$, satisfy (26), (27) and*

$$M(q_0)\rho_h(v_0) - f(v_0, q_0) = O(h) \tag{50}$$

where ρ_h is the corresponding discretization operator. Applying the CS and CM iterations to (42), the approximate Jacobian matrix for the CS iteration satisfies

$$\|J(q_0, v_0) - J(q^*, v^*)\| = \frac{\delta}{\epsilon}O(h) + O(h) \tag{51}$$

where $\delta = \|Bq_0 - Bq^*\|$, and $J(q, v)$ is the Jacobian of (42). For the CM iteration, we have

$$\|\bar{J}(q_0, v_0) - J(q^*, v^*)\| = O(h) \tag{52}$$

where $\bar{J}$ is the approximate Jacobian in the CM iteration.

Proof. The difference between the Jacobian at (q_0, v_0) and (q^*, v^*) can be written as

$$\|J_0 - J^*\| \leq \|P(q_0)\frac{\partial r}{\partial q}(q_0) - P(q^*)\frac{\partial r}{\partial q}(q^*)\| + \|\frac{dP}{dq}(q_0)r(q_0) - \frac{dP}{dq}(q^*)r(q^*)\| + O(h)$$

since the initial values satisfy (50). Under the conditions (26) and (27), we may choose common X and Y for $P(q_0)$ and $P(q^*)$ such that the first term on the right-hand side of the above inequality can be rewritten as

$$\|P(\hat{q})(\frac{\partial r}{\partial q}(q_0) - \frac{\partial r}{\partial q}(q^*))\| = O(h)$$

for some $\hat{q} \in [q_0, q^*]$, since $\frac{\partial r}{\partial q} = \frac{1}{\epsilon}B + O(h)$ allowing the cancellation of $\frac{1}{\epsilon}B$. The second term yields

$$\|\frac{dP}{dq}(q_0)r(q_0) - \frac{dP}{dq}(q^*)r(q^*)\| \leq \|r(q_0) - r(q^*)\|O(h) = \frac{1}{\epsilon}\|Bq_0 - Bq^*\|O(h)$$

according to Lemma 1. Thus, (51) is proved. Recalling $\bar{J}(q_0, v_0)$ from (16), we have

$$\|\bar{J}_0 - J^*\| \leq \|P\|\|\frac{\partial^2 r}{\partial q^2}\| = O(h),$$

using again Lemma 1. □

Theorem 4 *For the initial values (q_0, v_0), suppose the conditions in Lemma 3 hold. Suppose that the CS and the CM iterations are carried out by applying a simplified Newton method, where the iteration matrix is computed at the starting values (q_0, v_0). If both iterations converge, then the rate of convergence of the CS iteration $\sigma^{(CS)}$ compared to that of the CM iteration $\sigma^{(CM)}$ is given by*

$$\sigma^{(CS)} = \frac{\delta}{\epsilon}O(h) + O(h)$$

where $\delta = \|B(q_o - q^*)\|$, and

$$\sigma^{(CM)} = O(h).$$

Proof. We consider the rate of convergence that is defined by

$$\sigma = \limsup_{k\to\infty} \frac{\|q_{k+1} - q^*\|}{\|q_k - q^*\|}. \tag{53}$$

Since we apply the simplified Newton iteration, the solution of the CS iteration can be written as

$$\begin{bmatrix} q_{k+1} \\ v_{k+1} \end{bmatrix} = H(q_k, v_k)$$

where

$$H(q, v) = \begin{bmatrix} q \\ v \end{bmatrix} - J_0^{-1}F(q, v).$$

Similarly, the CM iteration can be written as the fixed-point iteration of the function

$$\bar{H}(q,v) = \begin{bmatrix} q \\ v \end{bmatrix} - \bar{J}_0^{-1} F(q,v).$$

Applying the Contractive Mapping Theorem, see [5] pp. 93-94, we obtain the rates of convergence of the CS and CM iterations:

$$\sigma^{CS} = \|I - J_0^{-1} J(q^*, v^*)\| = \|J_0^{-1}(J_0 - J^*)\|$$

and

$$\sigma^{CM} = \|I - \bar{J}_0^{-1} J(q^*, v^*)\| = \|\bar{J}_0^{-1}(\bar{J}_0 - J^*)\|$$

where $J(q^*, v^*) = J^*$ is the Jacobian at the solution of the discretized system, and the superscripts denote the respective iterations. For J_0^{-1}, we have

$$J_0 = \begin{bmatrix} \frac{\alpha}{h} + O(h) & -I \\ \frac{\delta}{\epsilon} B + O(h) & \frac{\alpha}{h} M + O(h) \end{bmatrix}.$$

When $\epsilon \to 0$, the dominant components of J_0^{-1} are of $O(1)$. From Lemma 3, the rates are

$$\sigma^{CS} = \frac{\delta}{\epsilon} O(h) + O(h)$$

and

$$\sigma^{CS} = O(h),$$

since $\bar{J}_0^{-1}$ has no component of $O(\frac{\delta}{\epsilon})$. □

In the stiff bushing example of [24], we have seen that the CM iteration was far more efficient than the CS iteration. The results match the prediction of Theorem 4, e.g., as $\epsilon \to 0$, the CS iteration became very ineffective due to failures in the convergence test for the Newton iterative solutions.

5 Example

An important class of applications of the CS and CM iterations is flexible multibody dynamics, which leads to the coupled large displacement-small deformation equations of motion [25, 16]. As shown schematically in Fig. 1, the deformation force between the ith and jth components is a function of the relative displacement of the reference frames X_i'-Y_i'-Z_i' and X_j'-Y_j'-Z_j'. Typically, the relative displacement is measured by

$$d_{ij} = r_j + A_j s_j' - r_i - A_i s_i' \tag{54}$$

where s_i' and s_j' are constant vectors to the origins of the force reference frames in their respective *local* coordinate systems, i.e., X_i-Y_i-Z_i and X_j-Y_j-Z_j, where r_i, r_j are the corresponding origins in a *global* coordinate system and A_i and A_j are the transformation matrices from the *global* to the *local* coordinate system [10]. The relative angles, $\Theta_{ij} = [\psi_{ij}, \theta_{ij}, \phi_{ij}]^T$, are calculated as

$$A_{ij} = (A_i B_i)^T A_j B_j$$
$$\psi_{ij} = -A_{ij}(2,3)$$
$$\theta_{ij} = A_{ij}(1,3)$$
$$\phi_{ij} = \arctan\left(\frac{A_{ij}(2,1)}{A_{ij}(2,2)}\right)$$

where $A_{ij}(k,l)$ is the component of the kth row and lth column of A_{ij}. The matrix A_{ij} is the relative orientation matrix of two force reference frames, i.e., B_i and B_j are constant. The relative velocity is the time derivative of the relative displacement $\dot{d}_{ij} = \frac{d}{dt} d_{ij}$ and relative angular velocity is $\omega_{ij} = \omega_j - \omega_i$, where ω_i and ω_j are angular velocities of body i and j, respectively.

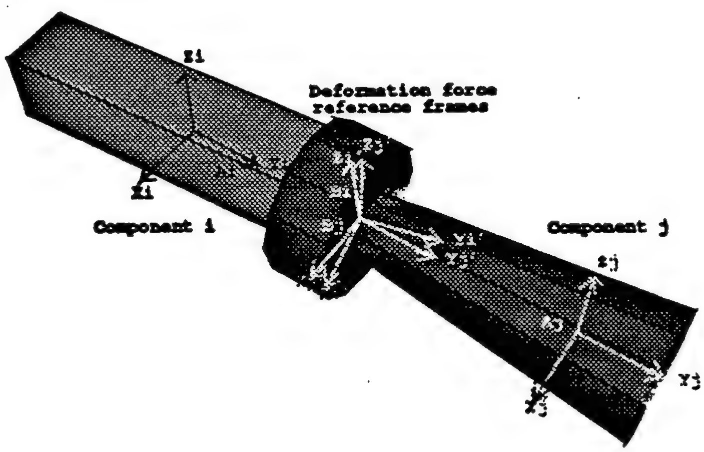

Figure 1: Deformation Force of a Flexible Body

Using the above defined notation, the force acting between the ith and jth components due to the deformation can be written as

$$f_{ij} = A_i B_i (K^f (A_i B_i)^T d_{ij} + C^f (A_i B_i)^T \dot{d}_{ij})$$

where K^f is a 3×3 structural stiffness matrix and C^f is the 3×3 damping coefficient matrix. Similarly, the torque acting between the components is

$$\tau_{ij} = A_i B_i (K^\tau \Theta_{ij} + C^\tau (A_i B_i)^T \omega_{ij})$$

where K^τ and C^τ are analogous to K^f and C^f. Note that the force and torque in this form are linear functions of the relative displacement (d_{ij}, Θ_{ij}) and the relative velocity $(\dot{d}_{ij}, \Omega_{ij})$.

To illustrate the deformation forces acting on bodies, we consider, in Cartesian coordinates (x, y, θ), a simplified 2D bushing force at the body-fixed coordinate frame, whose origin is $(-\frac{1}{2}, 0)$ and the axes are parallel to the body-fixed centroid frame. The other reference coordinate frame is fixed to the global position $(\frac{1}{2}, 0)$, whose axes are parallel to the global coordinate frame. The bushing force has stiffness matrix

$$K^f = \frac{1}{\epsilon} \begin{bmatrix} k^x & 0 & 0 \\ 0 & k^y & 0 \\ 0 & 0 & k^\theta \end{bmatrix}$$

where k^x, k^y, and k^θ are $O(1)$, and damping matrix

$$C^f = \begin{bmatrix} c^x & 0 & 0 \\ 0 & c^y & 0 \\ 0 & 0 & c^\theta \end{bmatrix}$$

where c^x, c^y, and c^θ are $O(1)$. For the 2D bushing example, (44) becomes

$$B(\theta) = \frac{1}{\epsilon} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & k^\theta \end{bmatrix} + |k^x - k^y| \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta & 0 \\ \cos\theta\sin\theta & \sin^2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

The kinematic constraints on the body are

$$\frac{1}{2}(x^2 + y^2 - l^c) = 0$$

and

$$\theta - \theta_0 = 0$$

where l^c is a constant. Let the gravity and the mass-inertia be unity, and $k^x = k^y = 1$, then the *equilibrium* of the bushing force satisfies

$$x = \frac{1}{2}(1 + \cos\theta_0)$$

$$y = \frac{1}{2}\sin\theta_0 - \epsilon$$

along with the constraint equations. For the equilibrium of this system to lie on the constraint manifold, we should have

$$l^\epsilon = \epsilon(\epsilon - \sin\theta_0) + \frac{1}{2}(1 + \cos\theta_0).$$

For simplicity, we consider the case $\theta_0 = 0$ and the corresponding l^ϵ such that the equilibrium $(1, -\epsilon, 0)$ of the bushing force lies on the constraint manifold. Near the equilibrium, we can choose the CS matrix as

$$P = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} - \begin{bmatrix} \frac{y}{\delta} \\ 0 \end{bmatrix}$$

since $x \approx 1$. Applying a numerical integration formula (such as BDF) to the CS formulation of the system yields

$$\begin{aligned}
\rho_h y - w - \frac{y}{x}(\rho_h x - v) &= 0 && \text{(55a)} \\
\rho_h w - f^y + 1 - \frac{y}{x}(\rho_h v - f^x) &= 0 && \text{(55b)} \\
xv + yw &= 0 && \text{(55c)} \\
\omega &= 0 && \text{(55d)} \\
\frac{1}{2}(x^2 + y^2 - l^\epsilon) &= 0 && \text{(55e)} \\
\theta &= 0 && \text{(55f)}
\end{aligned}$$

where the velocity is $[v, w, \omega]$, and the bushing force is

$$\begin{bmatrix} f^x \\ f^y \\ f^\theta \end{bmatrix} = B(\theta) \begin{bmatrix} \frac{1}{2} - x + \frac{1}{2}\cos\theta \\ -y + \frac{1}{2}\sin\theta \\ -\theta \end{bmatrix}.$$

Using the starting values $x_0 = 0.9$, $y_0 = -\sqrt{l^\epsilon - x_0^2}$, $\theta_0 = 0$, and the velocity $[-4.843 \times 10^{-3}, -1.0 \times 10^{-2}, 0]$, we obtain the results of the CS and CM iterations from DASSL [19] with various initial stepsize h_0 and the ending time at h_0. The solution tolerance TOL is set to 10^{-10}, and the stiffness $\epsilon = 10^{-5}$ and the damping factors $c^x = c^y = 10$. As shown in Table 1, using only the first-order Euler method, the CS and CM iterations are nearly identical for the initial stepsize h_0 ranging from 10^{-3} to 0.05. This is because δ is small due to the fact that the predictor is very accurate. The approximate rates of convergence of the two iterations when read in DASSL agree up to 7 digits at the termination, where the maximum allowed iterations per step in DASSL has been increased to 50. In Table 2, using initial stepsize $h_0 = 5.0 \times 10^{-3}$, starting values $x_0 = 0.8$, $y_0 = -\sqrt{l^\epsilon - x_0^2}$, $\theta_0 = 0$, and zero velocity vector, the CS and CM iterations are nearly identical as the solution TOL decreases from 10^{-4} to

Method	h_0	*no. iter.*	*approx. rate of convg.*
CS	10^{-3}	24	0.31602489817881
CM	10^{-3}	24	0.31602542368461
CS	5×10^{-3}	46	0.52240576939833
CM	5×10^{-3}	46	0.52240703666124
CS	10^{-2}	74	0.65889119756221
CM	10^{-2}	74	0.65889222379467
CS	5×10^{-2}	96	0.72329054568167
CM	5×10^{-2}	96	0.72329103128307

Table 1: Simplified 2D Bushing Force - Rates of Convergence for Nonlinear Iteration with Initial Stepsize h_0

Method	TOL	*step*	$f-s$	$j-s$	$etf-s$	$ctf-s$
CS	10^{-4}	17	79	17	3	1
CM	10^{-4}	17	79	17	3	1
CS	10^{-6}	17	130	17	2	2
CM	10^{-6}	17	129	17	2	2
CS	10^{-8}	13	146	11	0	2
CM	10^{-8}	13	147	11	0	2
CS	10^{-10}	13	175	11	0	2
CM	10^{-10}	13	176	11	0	2
CS	10^{-12}	13	200	11	0	2
CM	10^{-12}	13	202	11	0	2

Table 2: Simplified 2D Bushing Force - Results from DASSL in 0-0.05 Seconds Run

10^{-12} in the simplified bushing example using the first-order Euler method in DASSL. Because of the strong damping property of the backward Euler method, the solution converged to the fixed point $(1, -10^{-5}, 0)$ after the time $t = 0.05$ seconds.

We also examined the case where the bushing force continuously generates oscillatory forces so that the predictor may be far away from the smooth solution. Preloading the bushing force by moving the attachment points from $(\frac{1}{2}, 0)$ and $(-\frac{1}{2}, 0)$ to $(0, 0)$ on the global and the body-fixed frames, respectively, i.e., the bushing force becomes

$$\begin{bmatrix} f^x \\ f^y \\ f^\theta \end{bmatrix} = -B(\theta) \begin{bmatrix} x \\ y \\ \theta \end{bmatrix}.$$

For $q = (x, y, \theta)$ satisfying the constraints, the magnitude of the bushing force is $O(\frac{1}{\epsilon})$, since $\delta = \|q - q^*\| = O(1)$. Using the initial values $[1,0,0,0,0,0]$, $l^c = 1$, $TOL = 10^{-10}$, and $\epsilon = 10^{-5}$, Tab. 3 contains the results of the CS and CM iterations. To observe the behavior of Newton convergence, we have chosen the stepsize h_0 from 10^{-3} to 5×10^{-2} and ending time equal to h_0, with the order of BDF in DASSL restricted to one. For this test, DASSL was modified so that the number of Newton iteration per time step is ≤ 100 (instead of the default 4).

Under these conditions, the CS and CM iterations are recorded in Tab. 3. The rate of convergence of the CM iteration is commensurable to the stepsize, i.e., the number of function evaluations decreases when the stepsize is halved. For larger stepsizes, i.e., h_0 ranging from 0.005 to 0.00075, the CS iteration exhibits more frequent Jacobian changes than the CM iteration because of the error and convergence test failures in the CS iterations. Hence, more than one steps were taken when DASSL restarted with a smaller stepsize $\frac{h_0}{4}$. This agrees with the prediction given by Theorem 3, since the constrained potential force is of the same order of magnitude as the bushing force, i.e., $O(\frac{1}{\epsilon})$. The CS iteration performs much better for smaller h_0, e.g., from 0.0005 to 10^{-4}, than for larger h_0. This is because for $h \leq \sqrt{\epsilon}$, $\frac{\delta}{\epsilon} O(h^2) \approx O(h^2)$ for the forward Euler predictor. For the case $h_0 = 0.0001$, the CS iteration converged in one iteration.

In a full 2D bushing example, i.e., the two-body bi-directional force (44), which was preloaded as the simplified bushing, a large number of convergence test failures in the CS iterations was observed in Table 4. For this two-body model, we used $g = 13.5$, $l^c = 1$, $k^x = k^y = k^\theta = 10^{-5}$, and $c^x = c^y = c^\theta = 10$. Using the initial values $[0, 0, 0, 0, 0.9989, -0.001485, 0]$ and the initial velocity $[0, 0, 0, -0.675e-4, -0.45444e-2, 0]$, results from DASSL of a 0 to 0.5 second simulation are contained in Table 4. In this case, even when the position and velocity are within the TOL as shown in the last two columns in Tab. 3, $\frac{\delta}{\epsilon}$ can be large since the preloaded bushing may cause $\delta \gg \epsilon$.

Method	h_0	*step*	$f-s$	$j-s$	$etf-s$	$ctf-s$
CS	0.005	7	128	10	2	1
CM	0.005	1	57	1	0	0
CS	0.0025	9	80	9	2	1
CM	0.0025	1	20	1	0	0
CS	0.001	5	28	7	2	0
CM	0.001	1	8	1	0	0
CS	0.00075	9	52	12	5	0
CM	0.00075	1	6	1	0	0
CS	0.0005	8	26	4	2	0
CM	0.0005	1	4	1	0	0

Table 3: Preloaded Simplified 2D Bushing Force

Method	TOL	*step*	$f-s$	$j-s$	$etf-s$	$ctf-s$	x	v
CS	10^{-3}	125	465	147	19	28	0.8531799	-0.6712374
CM	10^{-3}	27	55	9	0	0	0.8527	-0.6431779
CS	10^{-4}	96	278	86	2	22	0.8528879	-0.6433484
CM	10^{-4}	35	72	11	1	0	0.8527338	-0.6447480
CS	10^{-5}	188	630	225	1	57	0.8527399	-0.6447200
CM	10^{-5}	45	94	7	0	0	0.8527340	-0.6447466
CS	10^{-6}	172	542	148	2	39	0.8527345	-0.6447471
CM	10^{-6}	60	122	8	1	0	0.8527342	-0.6447488

Table 4: Two-body 2D Bushing Force in 0-0.5 Seconds Run

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